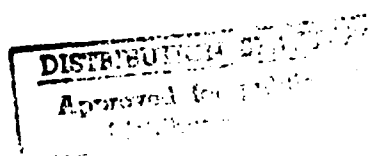


AD-A197 575

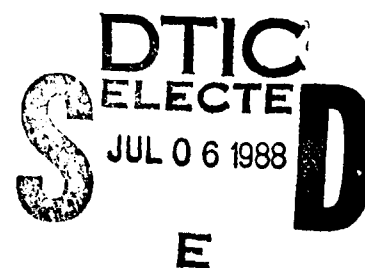
MULTIRESPONSE ROTABILITY

By

André I. Khuri
Department of Statistics
University of Florida
Gainesville, FL 32611



Technical Report Number 306
June 1988



Prepared Under Grant No. N00014-86-K-0059 From the Office of Naval Research,
André I. Khuri and Ramona C. Littell, Principal Investigators.

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 306	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Multiresponse Rotatability		5. TYPE OF REPORT & PERIOD COVERED
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Andre' I. Khuri		8. CONTRACT OR GRANT NUMBER(s) N00014-86-K-0059 R & T 4114552---01 Acct. No. 49101623459
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Statistics 476 Little Hall, University of Florida Gainesville, FL 32611		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Mathematical Sciences Division Arlington, VA 22217-5000		12. REPORT DATE June 1988
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		13. NUMBER OF PAGES 17
		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION, DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for Public Release: Distribution Unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Design moment; Multiresponse model; Rotatable design; Single-response model.		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This article introduces the concept of design rotatability in a multiresponse situation. Conditions for multiresponse rotatability are presented. These cause the prediction variances and covariances to be constant on spheres.		

MULTIRESPONSE ROTABILITY

André I. KHURI

Department of Statistics, University of Florida, Gainesville, FL 32611, USA

Abstract: Since its introduction by Box and Hunter (1957), rotatability of a response surface design has always been associated with single-response models. The present article extends this design concept to multiresponse models. For these models, rotatability means constant prediction variances and covariances, and hence correlations, among the predicted responses at points that are equidistant from the design center. It is shown that multiresponse rotatability can be achieved if and only if the design is rotatable (in the usual sense) for a single-response model whose order, or degree, is the highest among all the response models under consideration. This property does not depend on the form of the variance-covariance matrix of the responses.

AMS Subject Classification: Primary 62K99; Secondary 62J99.

Key words and phrases: Design moment; Multiresponse model; Prediction variances and covariances; Rotatable design; Single-response model.



Accession For	
NTIS GRA&I	<input checked="checked" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

1. Introduction

Box and Hunter (1957) proposed the idea of rotatability for a single-response model of the form

$$y = \underline{X}\underline{\beta} + \epsilon. \quad (1.1)$$

By definition, a design D for fitting model (1.1) is rotatable if the prediction variance, $\text{Var}[\hat{y}(\xi)]$, where $\hat{y}(\xi)$ is the predicted response at a point ξ , remains constant at all points that are equidistant from the design center. Equivalently, the quality of prediction, as measured by the size of the prediction variance, remains invariant to any rotation of the coordinate axes, if the design is rotatable. This is a desirable feature in a design, but is not an essential one. However, since rotatability, or near rotatability, can be easily achieved, it is rather insensible to work with a design that has a considerable deviation from rotatability. Draper and Guttman (1988) and Khuri (1988) proposed two different measures of rotatability to determine when a design is near rotatable.

In a multiresponse situation several responses are considered simultaneously. Suppose that we have a system of r response variables: y_1, y_2, \dots, y_r ; each of which depends on the same set of k input variables denoted by x_1, x_2, \dots, x_k within an experimental region A . The input variables are coded so that the design center is the point at the origin of the coordinates system. The model for the i^{th} response is

$$y_i(\xi) = \mu_i(\xi) + \epsilon_i, \quad i = 1, 2, \dots, r, \quad (1.2)$$

where $\mu_i(\xi)$ is a polynomial of degree d_i defined at $\xi = (x_1, x_2, \dots, x_k)'$ and ϵ_i is a random error ($i = 1, 2, \dots, r$). Model (1.2) can be expressed as

$$y_i(\xi) = \underline{x}'^{[d_i]} \underline{\beta}_i + \epsilon_i, \quad i = 1, 2, \dots, r, \quad (1.3)$$

where $\underline{x}' = (1, \xi')$, $\underline{x}'^{[d_i]}$ is the derived power vector of \underline{x}' of degree d_i , which consists of powers and cross products of powers of x_1, x_2, \dots, x_k with suitable multipliers such that $\underline{x}'^{[d_i]} \underline{x}^{[d_i]} = (\underline{x}' \underline{x})^{d_i}$ (see Box and Hunter, 1957, Section 5), and $\underline{\beta}_i$ is a vector of unknown parameters ($i = 1, 2, \dots, r$). The number of elements of $\underline{x}^{[d_i]}$ is p_i , where

$$p_i = \binom{k + d_i}{d_i}, \quad i = 1, 2, \dots, r. \quad (1.4)$$

If observations are made on the r responses at n design settings, then from (1.3) we obtain the models

$$\underline{y}_i = \underline{X}_i \underline{\beta}_i + \underline{\epsilon}_i, \quad i = 1, 2, \dots, r, \quad (1.5)$$

where \underline{y}_i and $\underline{\epsilon}_i$ are the vectors of observations and random errors, respectively, for the i^{th} response, and \underline{X}_i is of order $n \times p_i$ and rank p_i ($i = 1, 2, \dots, r$). It is assumed that

$$E(\underline{\epsilon}_i) = 0, \quad i = 1, 2, \dots, r, \quad (1.6)$$

$$E(\underline{\epsilon}_i \underline{\epsilon}_j') = \sigma_{ij} \underline{I}_n, \quad i, j = 1, 2, \dots, r, \quad (1.7)$$

where \underline{I}_n is the identity matrix of order $n \times n$. The models in (1.5) can be displayed as a single multiresponse model of the form

$$\underline{y}_m = \underline{X}_m \underline{\beta}_m + \underline{\epsilon}_m, \quad (1.8)$$

where $\underline{y}_m = (y'_1, y'_2, \dots, y'_r)'$, $\underline{\beta}_m = (\beta'_1, \beta'_2, \dots, \beta'_r)'$, $\underline{\epsilon}_m = (\epsilon'_1, \epsilon'_2, \dots, \epsilon'_r)'$, and X_m is the block-diagonal matrix, $\text{diag} (X_1, X_2, \dots, X_r)$. By (1.6) and (1.7), the variance-covariance matrix of $\underline{\epsilon}_m$ is $\Sigma \otimes I_n$, where $\Sigma = (\sigma_{ij})$ is the variance-covariance matrix of the responses of order $r \times r$ and \otimes is the direct, or Kronecker, product symbol. The best linear unbiased estimator of $\underline{\beta}_m$ is

$$\hat{\underline{\beta}}_m = \left[X'_m (\Sigma^{-1} \otimes I_n) X_m \right]^{-1} X'_m (\Sigma^{-1} \otimes I_n) \underline{y}_m. \quad (1.9)$$

The variance-covariance matrix of $\hat{\underline{\beta}}_m$ is given by

$$\text{Var}(\hat{\underline{\beta}}_m) = \left[X'_m (\Sigma^{-1} \otimes I_n) X_m \right]^{-1}. \quad (1.10)$$

Let $\hat{\underline{y}}_m(\xi)$ be the $r \times 1$ vector of predicted responses at a point ξ in the region A , that is,

$$\hat{\underline{y}}_m(\xi) = [\hat{y}_1(\xi), \hat{y}_2(\xi), \dots, \hat{y}_r(\xi)]', \quad (1.11)$$

where

$$\hat{y}_i(\xi) = x^{[d_i]} \hat{\beta}_i, \quad i = 1, 2, \dots, r, \quad (1.12)$$

and $\hat{\beta}_i$ is the best linear unbiased estimator of β_i obtained from (1.9). Formula (1.11) can then be written as

$$\hat{\underline{y}}_m(\xi) = \Lambda'(\xi) \hat{\underline{\beta}}_m, \quad (1.13)$$

where $\Lambda(\xi) = \text{diag} (x^{[d_1]}, x^{[d_2]}, \dots, x^{[d_r]})$. From (1.10) and (1.13) the variance-covariance matrix of $\hat{\underline{y}}_m(\xi)$ is equal to

$$\text{Var}[\hat{y}_m(\xi)] = \Lambda'(\xi) \left[X_m' (\Sigma^{-1} \otimes I_n) X_m \right]^{-1} \Lambda(\xi). \quad (1.14)$$

Definition 1.1. A design D for fitting the multiresponse model in (1.8) is said to be rotatable if $\text{Var}[\hat{y}_m(\xi)]$ is constant at all points, ξ , that are equidistant from the origin.

This definition is equivalent to stating that, when the design is rotatable, the variances and covariances of the predicted responses are constant on spheres (hyperspheres, in general) centered at the origin. This implies that the $r(r-1)/2$ correlations among the predicted responses are also constant on such spheres. The same thing can be said about the variance of any linear combination, $\sum_{i=1}^r c_i \hat{y}_i(\xi)$, of the predicted responses. This is a desirable feature since certain linear combinations of the responses may be of special interest to the experimenter. For example, it may be experimentally difficult to obtain independent measurements on some response. If, however, this response is linearly related to the other responses (because of physical or chemical laws), then its value can be determined in terms of the other responses (see Box et al., 1973, Section 6).

2. Conditions for Multiresponse Rotatability

Let ξ and η be two points that are the same distance from the origin. There is an orthogonal matrix, T , of order $k \times k$ such that $\eta = T\xi$. Let $z = (1, \eta')'$, then $z = Rx$, where $x = (1, \xi')'$ and

$$R = \text{diag} \left(1, T \right). \quad (2.1)$$

The matrix R is orthogonal of order $(k+1) \times (k+1)$. The derived power vector of degree d_i of z is of the form

$$z^{[d_i]} = R x^{[d_i]} x^{[d_i]}, \quad i = 1, 2, \dots, r. \quad (2.2)$$

where $R^{[d_i]}$ is the d_i th Schläflian matrix of R of order $p_i \times p_i$ and p_i is defined in (1.4). See, for example, Box and Hunter (1957, Section 5) for more details concerning Schläflian matrices. It is known that $R^{[d_i]}$ is an orthogonal matrix since R is. The vectors of predicted responses at ξ and η are $\hat{y}_m(\xi)$ and $\hat{y}_m(\eta)$, respectively. The variance-covariance matrix of $\hat{y}_m(\xi)$ is given in (1.14). Similarly, the variance-covariance matrix of $\hat{y}_m(\eta)$ can be written as

$$\text{Var} [\hat{y}_m(\eta)] = \Lambda'(\eta) \left[X_m' (\Sigma^{-1} \odot I_n) X_m \right]^{-1} \Lambda(\eta), \quad (2.3)$$

where $\Lambda(\eta) = \text{diag} (z^{[d_1]}, z^{[d_2]}, \dots, z^{[d_r]})$. Using the transformation (2.2), formula (2.3) can be rewritten as

$$\begin{aligned} \text{Var} [\hat{y}_m(\eta)] &= \Lambda'(\xi) S' \left[X_m' (\Sigma^{-1} \otimes I_n) X_m \right]^{-1} S \Lambda(\xi) \\ &= \Lambda'(\xi) \left[S' X_m' (\Sigma^{-1} \odot I_n) X_m S \right]^{-1} \Lambda(\xi), \end{aligned} \quad (2.4)$$

where S is the orthogonal matrix,

$$S = \text{diag} (R^{[d_1]}, R^{[d_2]}, \dots, R^{[d_r]}). \quad (2.5)$$

By Definition 1.1, multiresponse rotatability requires that the terms on the right sides of (1.14) and (2.4) be equal for all ξ and R . Since Σ is an arbitrary variance-covariance matrix, this equality should also hold for all positive definite matrices, Σ , of order $r \times r$. Now, $X_m' (\Sigma^{-1} \odot I_n) X_m$ and $S' X_m' (\Sigma^{-1} \odot I_n) X_m S$ can be partitioned as

$$X'_m (\Sigma^{-1} \otimes I_n) X_m = (\sigma^{ij} X'_i X_j)$$

$$S' X'_m (\Sigma^{-1} \otimes I_n) X_m S = \left(\sigma^{ij} R'^{[d_i]} X'_i X_j R^{[d_j]} \right),$$

where σ^{ij} is the $(i,j)^{th}$ element of Σ^{-1} . In order to achieve multiresponse rotatability we must therefore have

$$X'_i X_j = R'^{[d_i]} X'_i X_j R^{[d_j]}, \quad i, j = 1, 2, \dots, r, \quad (2.6)$$

for every orthogonal matrix, R , of the form given in (2.1).

Now, let t be the vector $(1, t_1, t_2, \dots, t_k)'$. Its derived power vector of degree d_i is $t^{[d_i]}$ ($i = 1, 2, \dots, r$). Consider the expression

$$Q_{ij} = t'^{[d_i]} X'_i X_j t^{[d_j]}, \quad i, j = 1, 2, \dots, r. \quad (2.7)$$

Note that

$$\begin{aligned} X_j t^{[d_j]} &= \left(x'_1{}^{[d_j]} t^{[d_j]}, x'_2{}^{[d_j]} t^{[d_j]}, \dots, x'_n{}^{[d_j]} t^{[d_j]} \right)' \\ &= \left[(x'_1 t)^{d_j}, (x'_2 t)^{d_j}, \dots, (x'_n t)^{d_j} \right]', \quad j = 1, 2, \dots, r, \end{aligned} \quad (2.8)$$

where $x'_u = (1, \xi'_u)$ and ξ'_u is the vector of u^{th} design settings for the input variables ($u = 1, 2, \dots, n$). Formula (2.7) can then be written as

$$Q_{ij} = \sum_{u=1}^n \left(x'_{u1} t_1 \right)^{d_i+d_j}$$

$$= \sum_{u=1}^n \left(1 + \sum_{l=1}^k x_{ul} t_l \right)^{d_i+d_j}, \quad i, j = 1, 2, \dots, r, \quad (2.9)$$

where x_{ul} is the value of the l^{th} input variable at the u^{th} experimental run ($l = 1, 2, \dots, k$; $u = 1, 2, \dots, n$). By applying the multinomial expansion to (2.9) it can be verified that the coefficient of $t_1^{\delta_1} t_2^{\delta_2} \dots t_k^{\delta_k}$ in this expansion is

$$\frac{(d_i + d_j)!}{\prod_{l=1}^k (\delta_l)! (d_i + d_j - \delta)!} (1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k}), \quad i, j = 1, 2, \dots, r, \quad (2.10)$$

where $\delta_1, \delta_2, \dots, \delta_k$ are nonnegative integers such that $\delta = \sum_{l=1}^k \delta_l \leq d_i + d_j$, and $(1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k})$ is a design moment of order δ defined as

$$(1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k}) = \sum_{u=1}^n x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k}. \quad (2.11)$$

The quantity Q_{ij} is therefore a generating function for the design moments through order $d_i + d_j$ ($i, j = 1, 2, \dots, r$). If the design is rotatable, then from (2.6) and (2.7) we obtain

$$Q_{ij} = t'^{[d_i]} R'^{[d_i]} X'_i X_j R^{[d_j]} t^{[d_j]}$$

$$= (t' R')^{[d_i]} X'_i X_j (R t)^{[d_j]}, \quad i, j = 1, 2, \dots, r. \quad (2.12)$$

Thus, Q_{ij} remains unchanged by any orthogonal transformation of t of the form (2.1) if and only if the design is rotatable. Since Q_{ij} is a polynomial of degree $d_i + d_j$ in t_1, t_2, \dots, t_k , it must be a function of $\sum_{l=1}^k t_l^2$, that is,

$$Q_{ij} = \sum_{s=0}^{e_{ij}} a_{2s}^{ij} \left(\sum_{l=1}^k t_l^2 \right)^s, \quad i, j = 1, 2, \dots, r, \quad (2.13)$$

where $e_{ij} = [(d_i + d_j)/2]$ is the greatest integer in $(d_i + d_j)/2$. The coefficient of $t_1^{\delta_1} t_2^{\delta_2} \dots t_k^{\delta_k}$ in (2.13) is, therefore, zero if any of the δ_l ($l = 1, 2, \dots, k$) are odd integers. If all the δ_l are even, then the coefficient is

$$\frac{a_{\delta}^{ij} (\delta/2)!}{\prod_{l=1}^k (\delta_l/2)!}, \quad \delta = \sum_{l=1}^k \delta_l \leq d_i + d_j, \quad i, j = 1, 2, \dots, r. \quad (2.14)$$

By comparing (2.10) with (2.14) it can be concluded that a design is rotatable if and only if the design moments through order $d_i + d_j$ ($i, j = 1, 2, \dots, r$) are of the form

0, if any δ_l is odd

$$\left(t_1^{\delta_1} t_2^{\delta_2} \dots t_k^{\delta_k} \right) = \quad (2.15)$$

$$\frac{\lambda_{\delta}^{ij} \prod_{l=1}^k (\delta_l)!}{2^{\delta/2} \prod_{l=1}^k (\delta_l/2)!}, \quad \text{if all the } \delta_l \text{ are even,}$$

where λ_{δ}^{ij} is the quantity

$$\lambda_{\delta}^{ij} = \frac{a_{\delta}^{ij} 2^{\delta/2} (\delta/2)! (d_i + d_j - \delta)!}{(d_i + d_j)!}. \quad (2.16)$$

Since (2.15) must hold for all i, j ($= 1, 2, \dots, r$), it follows that the moments through order $2d$, where

$d = \max_{1 \leq \alpha \leq r} (d_{\alpha})$, of a rotatable design must be of the form

0, if any δ_l is odd

$$\left(1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k}\right) = \quad (2.17)$$

$$\frac{\lambda_\delta \prod_{l=1}^k (\delta_l)!}{2^{\delta/2} \prod_{l=1}^k (\delta_l/2)!}, \text{ if all the } \delta_l \text{ are even,}$$

where $\delta = \sum_{l=1}^k \delta_l \leq 2d$, and λ_δ is given by

$$\lambda_\delta = \frac{a_\delta 2^{\delta/2} (\delta/2)! (2d - \delta)!}{(2d)!}, \quad (2.18)$$

where a_δ is the value of a_δ^{ij} in (2.16), which corresponds to $i = j = i^*$ and i^* is such that $d_{i^*} = d = \max_{1 \leq \alpha \leq r} (d_\alpha)$.

On the basis of (2.17) it can finally be concluded that the necessary and sufficient condition to achieve multiresponse rotatability is that the design be rotatable for a single-response model of order $d = \max_{1 \leq \alpha \leq r} (d_\alpha)$.

3. Examples

Example 1. Consider a multiresponse system consisting of the three response models

$$y_1 = \beta_{10} + \beta_{11}x_1 + \beta_{12}x_2 + \beta_{13}x_3 + \epsilon_1$$

$$y_2 = \beta_{20} + \beta_{21}x_1 + \beta_{22}x_2 + \beta_{23}x_3 + \epsilon_2$$

$$y_3 = \beta_{30} + \sum_{i=1}^3 \beta_{3i} x_i + \sum_{i < j} \beta_{3ij} x_i x_j + \sum_{i=1}^3 \beta_{3ii} x_i^2 + \epsilon_3.$$

Here, $k = 3$, $r = 3$, $d_1 = d_2 = 1$, $d_3 = 2$, hence $d = 2$. The variance-covariance matrix of the responses is assumed to be

$$\Sigma = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 3 & 2 \\ 0 & 2 & 5 \end{bmatrix}. \quad (3.1)$$

The models are fitted using the design D given in Table 1. This is a second-order rotatable central composite design with one center point. By (2.17), D is also rotatable in the multiresponse sense. Using formula (1.14) it can be verified that

$$\text{Var}[\hat{y}_1(\xi)] = .1333 + .1464 \rho^2 \quad (3.2)$$

$$\text{Var}[\hat{y}_2(\xi)] = .20 + .2197 \rho^2 \quad (3.3)$$

$$\text{Var}[\hat{y}_3(\xi)] = 3.4671 - 1.9285 \rho^2 + .5617 \rho^4 \quad (3.4)$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_2(\xi)] = .0667 + .0732 \rho^2 \quad (3.5)$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_3(\xi)] = 0 \quad (3.6)$$

$$\text{Cov}[\hat{y}_2(\xi), \hat{y}_3(\xi)] = .1333 + .1464 \rho^2, \quad (3.7)$$

where $\rho^2 = x_1^2 + x_2^2 + x_3^2$. Thus, the variances and covariances of the three predicted responses are

constant on spheres centered at the origin.

To demonstrate that multiresponse rotatability does not depend on the form of Σ , another value of this matrix is now used, namely,

$$\Sigma = \begin{bmatrix} 3 & 5 & 1 \\ 5 & 9 & 3 \\ 1 & 3 & 4 \end{bmatrix}.$$

Formulas (3.2) - (3.7) become

$$\text{Var}[\hat{y}_1(\xi)] = .20 + .2197 \rho^2$$

$$\text{Var}[\hat{y}_2(\xi)] = .60 + .659 \rho^2$$

$$\text{Var}[\hat{y}_3(\xi)] = 1.1884 - .3819 \rho^2 + .1652 \rho^4$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_2(\xi)] = .3333 + .3661 \rho^2$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_3(\xi)] = .0667 + .0732 \rho^2$$

$$\text{Cov}[\hat{y}_2(\xi), \hat{y}_3(\xi)] = .20 + .2197 \rho^2.$$

Example 2. Consider again the three-response system as in Example 1, except that y_2 is now represented by the second-order model

$$y_2 = \beta_{20} + \sum_{i=1}^3 \beta_{2i} x_i + \sum_{i < j} \beta_{2ij} x_i x_j + \sum_{i=1}^3 \beta_{2ii} x_i^2 + \epsilon_2.$$

The design D and the variance-covariance matrix Σ are the same as in Table 1 and formula (3.1), respectively. In this case, the variances and covariances of the three predicted responses are

$$\text{Var}[\hat{y}_1(\xi)] = .1333 + .1464 \rho^2$$

$$\text{Var}[\hat{y}_2(\xi)] = 2.5042 - 1.4675 \rho^2 + .413 \rho^4$$

$$\text{Var}[\hat{y}_3(\xi)] = 4.9418 - 3.0083 \rho^2 + .8261 \rho^4$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_2(\xi)] = .0667 + .0732 \rho^2$$

$$\text{Cov}[\hat{y}_1(\xi), \hat{y}_3(\xi)] = 0$$

$$\text{Cov}[\hat{y}_2(\xi), \hat{y}_3(\xi)] = 1.9767 - 1.2034 \rho^2 + .3304 \rho^4.$$

4. Concluding Remarks

- i) In practice, the variance-covariance matrix Σ of the responses is unknown. Hence, the estimator $\hat{\beta}_m$ in (1.9) and its variance-covariance matrix given in (1.10) cannot be computed. An estimator of Σ is therefore needed. There are several possible estimators, two of which are given below (see Srivastava and Giles, 1987, Section 2.3)

$$\hat{\Sigma} = (\hat{\sigma}_{ij}) \tag{4.1}$$

$$\hat{\Sigma} = (\tilde{\sigma}_{ij}), \tag{4.2}$$

where

$$\hat{\sigma}_{ij} = y_i' \left[I_n - X_i(X_i'X_i)^{-1} X_i' \right] \left[I_n - X_j(X_j'X_j)^{-1} X_j' \right] y_j / n \quad (4.3)$$

$$\tilde{\sigma}_{ij} = y_i' \left[I_n - X(X'X)^{-1} X' \right] y_j / n, \quad (4.4)$$

where X is the matrix for a single-response model of order $d = \max_{1 \leq \alpha \leq r} (d_\alpha)$. The first estimator was proposed by Zellner (1962). If Σ is substituted by $\hat{\Sigma}$ and $\tilde{\Sigma}$ in (1.9), we get the estimators

$$\hat{\beta}_{ms} = \left[X_m' (\hat{\Sigma}^{-1} \otimes I_n) X_m \right]^{-1} X_m' (\hat{\Sigma}^{-1} \otimes I_n) y_m \quad (4.5)$$

$$\tilde{\beta}_{ms} = \left[X_m' (\tilde{\Sigma}^{-1} \otimes I_n) X_m \right]^{-1} X_m' (\tilde{\Sigma}^{-1} \otimes I_n) y_m, \quad (4.6)$$

respectively. Substituting these estimators for $\hat{\beta}_m$ in (1.13) leads to the predicted response vectors $\hat{y}_{ms}(\xi)$ and $\tilde{y}_{ms}(\xi)$, respectively.

The true variance-covariance matrices of $\hat{\beta}_{ms}$ and $\tilde{\beta}_{ms}$ are, to order $O(n^{-1})$, asymptotically equal to the variance-covariance matrix of $\hat{\beta}_m$, which is given in (1.10). See Srivastava and Giles (1987, Section 3.3). Approximate expressions for $\text{Var}[\hat{y}_{ms}(\xi)]$ and $\text{Var}[\tilde{y}_{ms}(\xi)]$ can then be obtained from (1.14) by substituting Σ by $\hat{\Sigma}$ and $\tilde{\Sigma}$, respectively. Hence, for large n these expressions are almost constant on spheres centered at the origin, if the design is rotatable.

- ii) The constancy of prediction variances and covariances on spheres when the design is rotatable results in constant correlations among the predicted responses. This interesting property is particularly useful for simultaneous inference making involving the responses. It would be quite discomforting if such inference were to change by a mere rotation of the coordinate axes.

which can occur in the absence of multiresponse rotatability.

Acknowledgements

This research was partially supported by the Office of Naval Research under Grant N00014-86-K-0059.

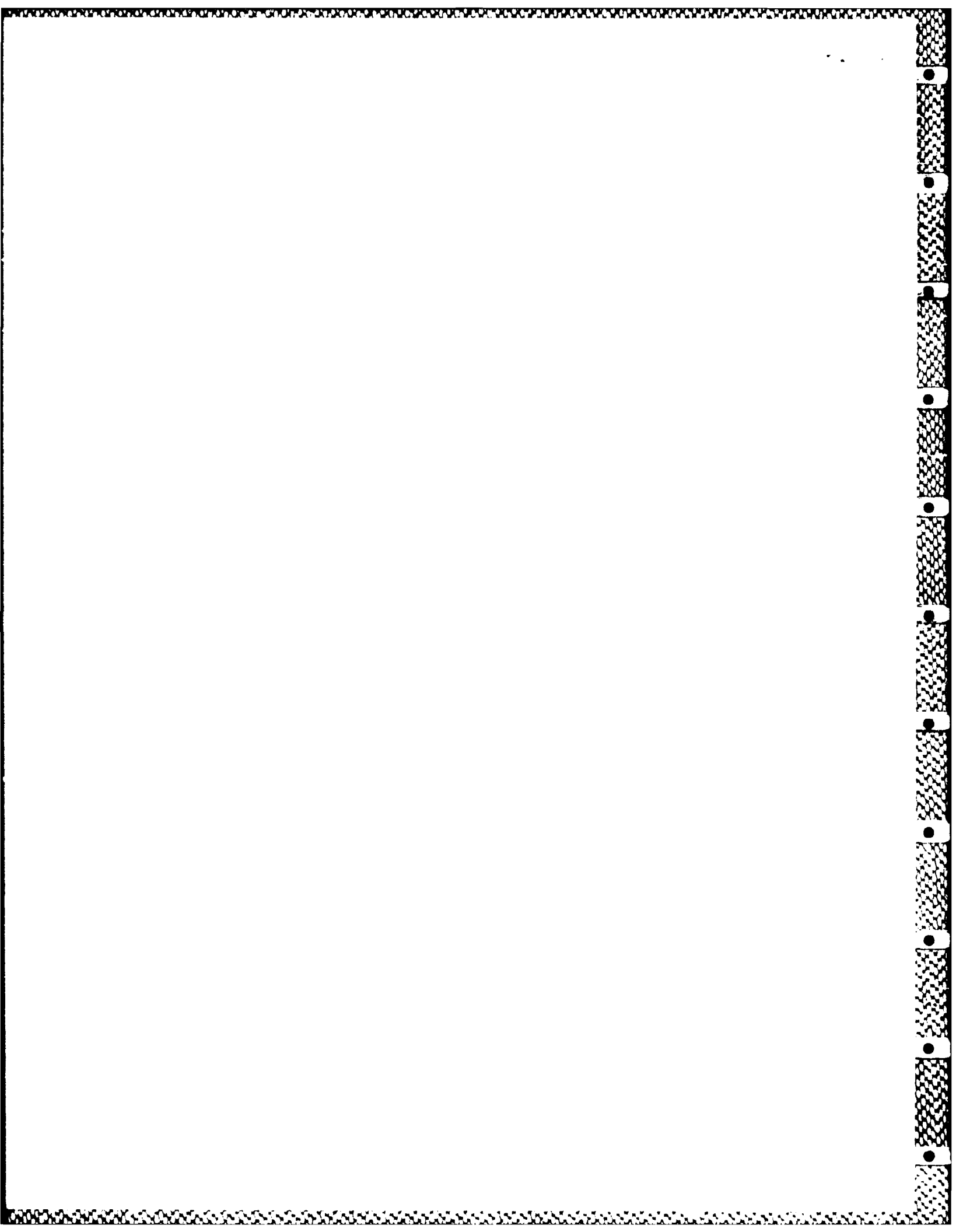
References

- Box, G.E.P. and J.S. Hunter (1957). Multi-factor experimental designs for exploring response surfaces. Annals of Mathematical Statistics 28, 195-241.
- Box, G.E.P., W.G. Hunter, J.F. MacGregor and J. Erjavec (1973). Some problems associated with the analysis of multiresponse data. Technometrics 15, 33-51.
- Draper, N.R. and I. Guttman (1988). An index of rotatability. Technometrics 30, 105-111.
- Khuri, A.I. (1988). A measure of rotatability for response-surface designs. Technometrics 30, 95-104.
- Srivastava, V.K. and D.E.A. Giles (1987). Seemingly Unrelated Regression Equations Models. Marcel Dekker, New York.
- Zellner, A. (1962). An efficient method of estimating seemingly unrelated regressions and tests for aggregation bias. Journal of the American Statistical Association 57, 348-368.

Table 1

The design points for Example 1

x_1	x_2	x_3
-1.0	-1.0	-1.0
1.0	-1.0	-1.0
-1.0	1.0	-1.0
-1.0	-1.0	1.0
1.0	1.0	-1.0
1.0	-1.0	1.0
-1.0	1.0	1.0
1.0	1.0	1.0
1.6818	0.0	0.0
-1.6818	0.0	0.0
0.0	1.6818	0.0
0.0	-1.6818	0.0
0.0	0.0	1.6818
0.0	0.0	-1.6818
0.0	0.0	0.0



END

DATE

FILMED

DTIC

9-88